Advanced Scientific Computing Research Program

Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment Program

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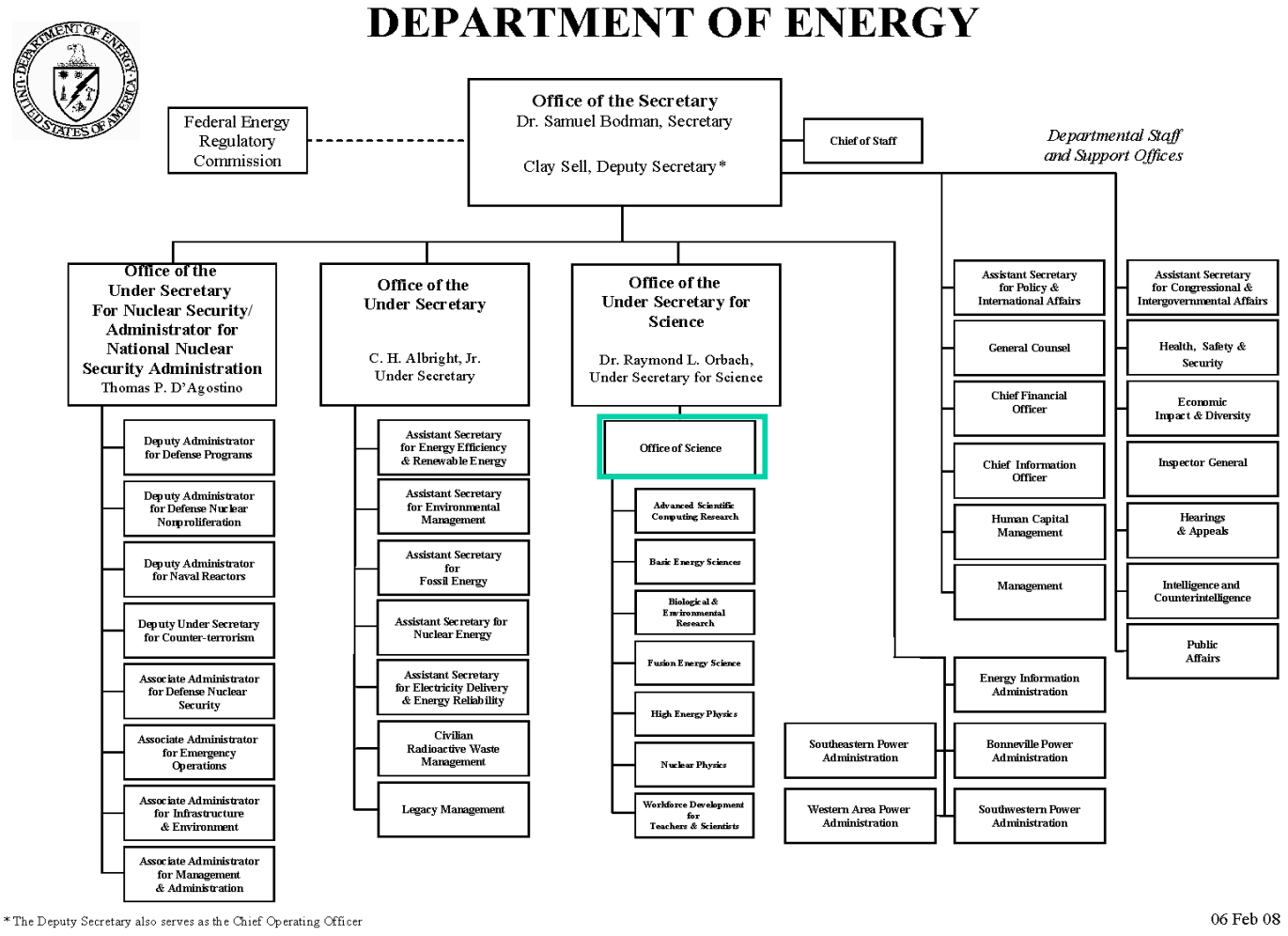
U.S. Department of Energy

Office of Science

Department of Energy Organizational Structure

Advanced Scientific Computing Research Program



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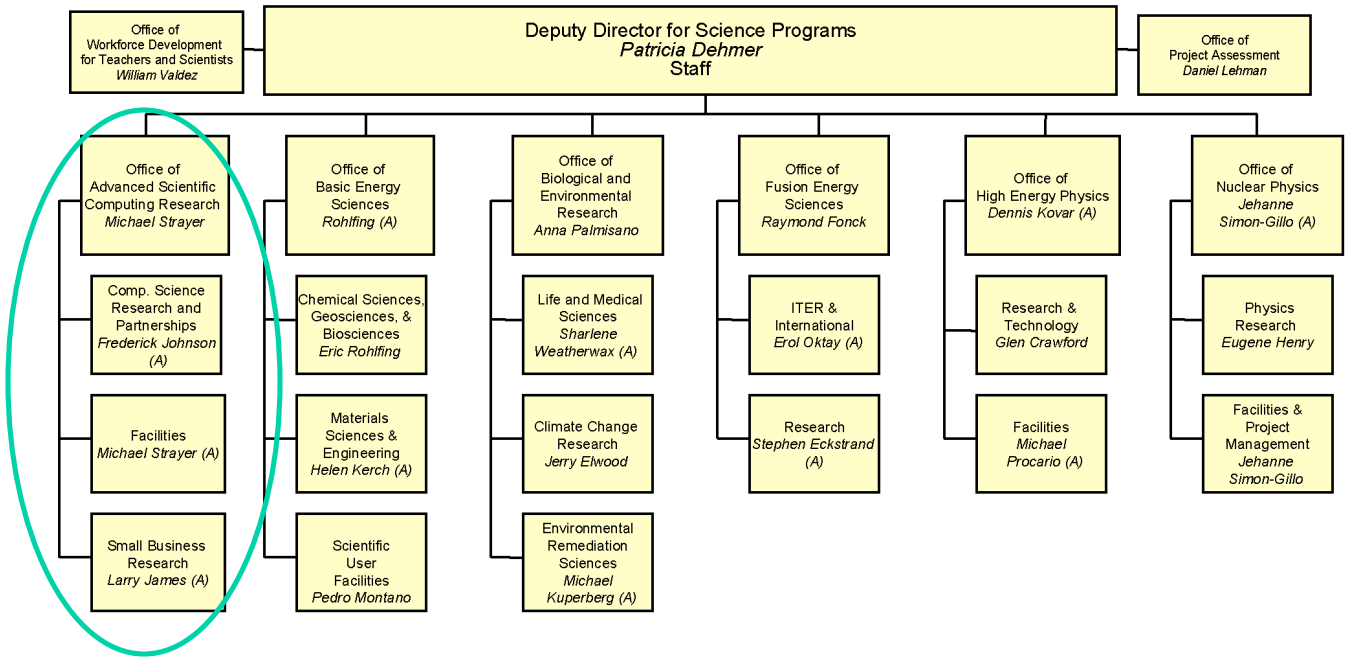
Advanced Scientific Computing Research Program



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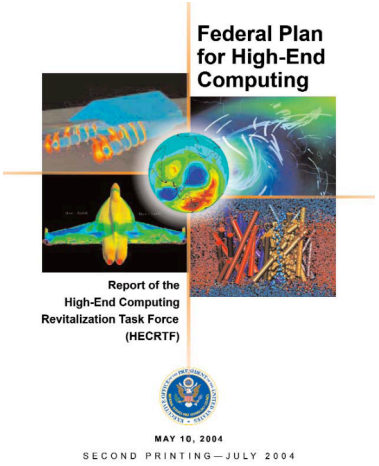
ASCR High Performance Computing Resources

Advanced Scientific Computing Research Program

- High Performance Production Computing Facility (NERSC)
  - Delivers high-end capacity computing to entire DOE SC research community
  - Large number of projects (200 – 300)
  - Medium- to very-large-scale projects that occasionally need a very high capability
  - Annual allocations

- Leadership Computing Facilities
  - Delivers highest computational capability to national and international researchers through peer-reviewed **Innovative and Novel Computational Impact on Theory and Computation (INCITE)** program
  - Small number of projects (10 – 20)
  - Multiple year allocations



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ASCR High Performance and Leadership Computing Facilities

Advanced Scientific Computing Research Program

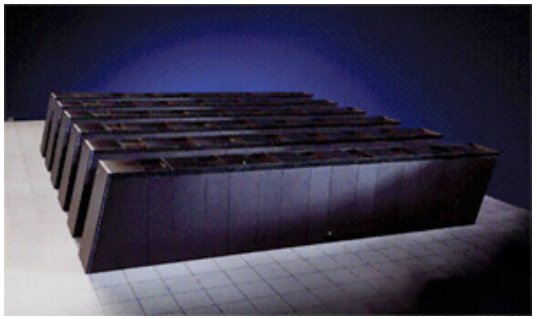
- NERSC
  - 104 teraflop Cray XT4 began operations in January 2008
  - 6.7 Teraflop IBM Power 5 (Bassi) with 888 processors, 3.5 terabytes aggregate memory
  - 3.1 Teraflop LinuxNetworx Opteron cluster (Jacquard) with 712 processors, 2.1 terabytes aggregate memory

- LCF at Oak Ridge
  - 119 teraflop Cray XT3/XT4 (Jaguar) with 11,708 dual core AMD Opteron processor nodes, 46 terabytes aggregate memory
  - 18.5 Teraflop Cray X1E (Phoenix) with 1,024 multi-streaming vector processors,

- Argonne LCF
  - 5.7 Teraflop IBM Blue Gene/L (BGL) with 2,048 PPC processors
  - 100 teraflop IBM Blue Gene/P began operations April 1, 2008

Future Facility Upgrades

- ALCF
  - 446 teraflop IBM Blue Gene/P upgrade in transition to operations



- LCF – Oak Ridge
  - Cray XT4 250 TF upgrade completed and acceptance testing due to start
  - 1 Petaflop Cray Baker system to be delivered by end of 2008

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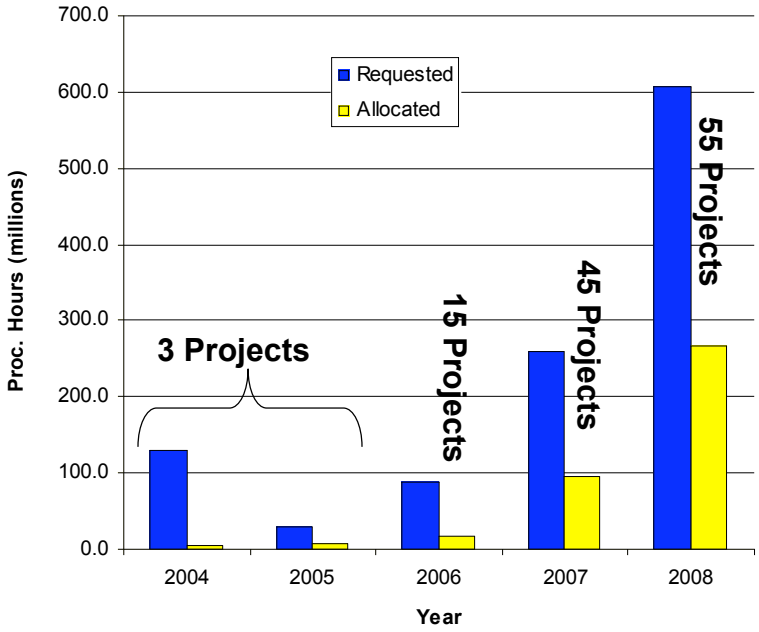
Innovative and Novel Computational Impact on Theory and Experiment- INCITE

Advanced Scientific Computing Research Program

- Initiated in 2004 at NERSC
- Provides Office of Science computing resources to a small number of computationally intensive research projects of large scale, that can make high-impact scientific advances through the use of a large allocation of computer time and data storage
- Open to national and international researchers, including industry
- No requirement of DOE Office of Science funding
- Peer and computational readiness reviewed



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2008 INCITE Awards: Allocations by Discipline

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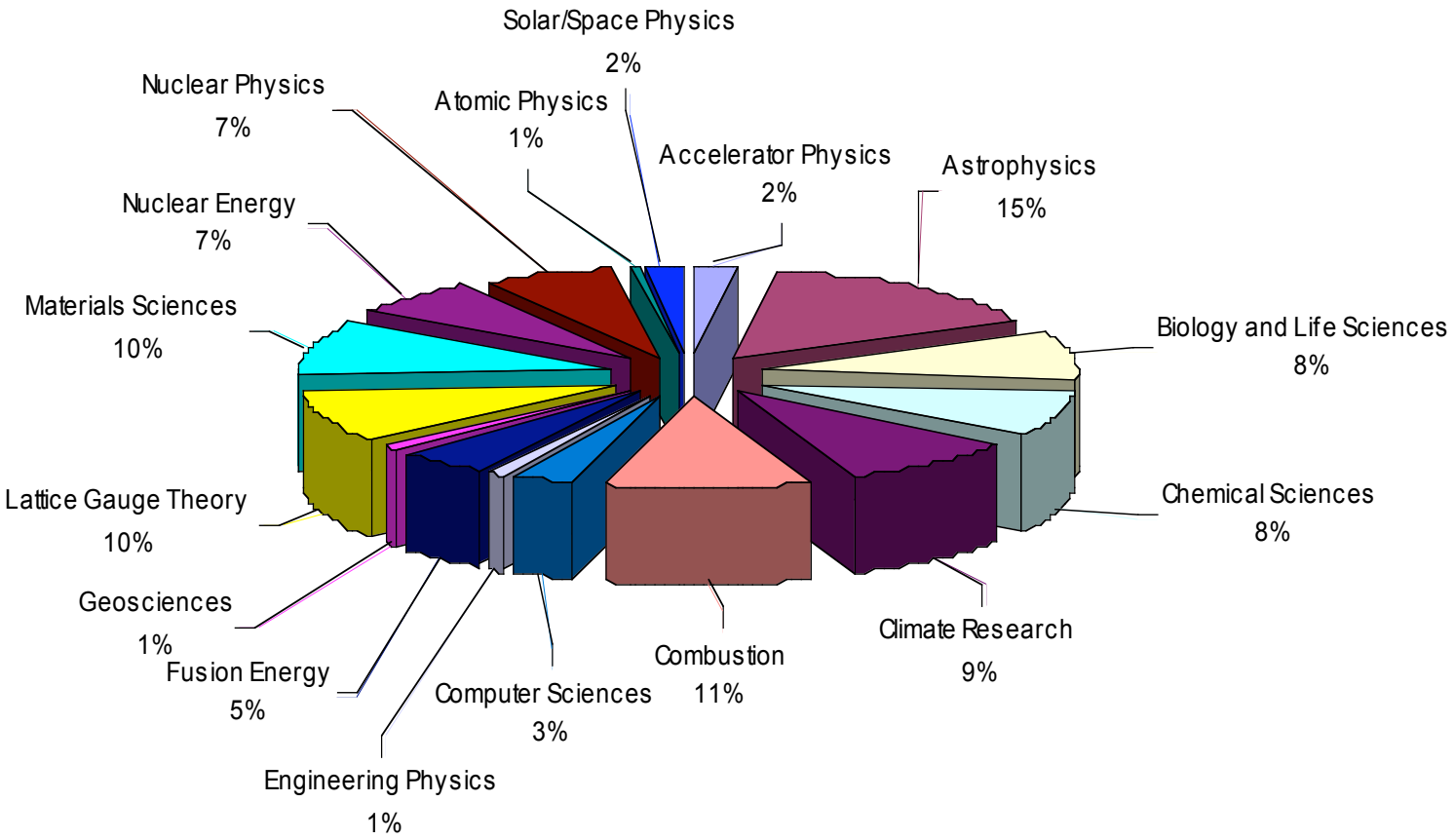

INCITE Expectations

- LCF
  - Sign LCF User Agreements
  - Adhere to LCF Cyber Security and other computing policies
  - Work with Scientific Computing Group to take full advantage of Jaguar and Phoenix architectures
  - Don’t wait until December to start computing
- DOE
  - If your project has a multiple year allocation, fill out renewal form
  - If this is your last year of project’s allocation, submit final report
  - Share your scientific accomplishments.

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2007 INCITE Accomplishments at ORNL

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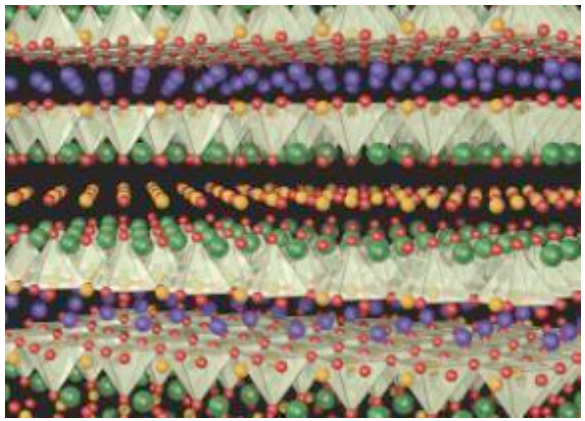
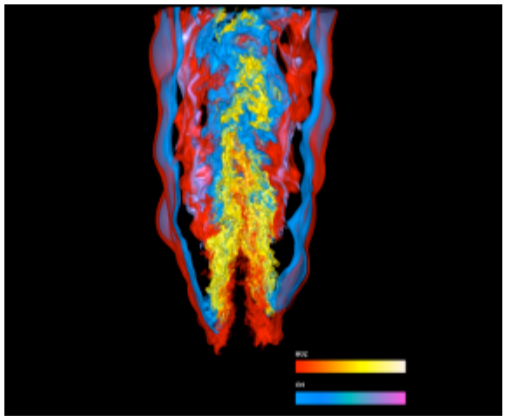
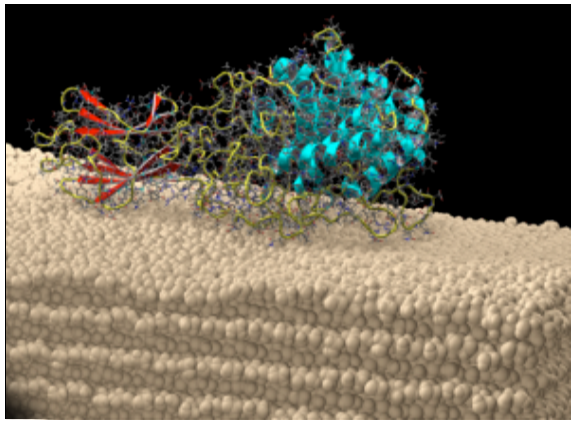


Resolved decades-long controversy about modeling physics of high temperature superconducting cuprates



First 3-D simulation of flame that resolves chemical composition, temperature, and flow



New insights into protein structure and function leading to better understanding of cellulose-to-ethanol conversion

2008 Scientific Accomplishments